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Comparison of Models for Fluorine Effect on Dopant Diffusion in CMOS Processes

I. INTRODUCTION

Recently a new diffusion model was introduced to Victory Process: the CMOS model. This model aims at taking on the challenges brought by the specificities of CMOS device processing such as steep temperature ramps, short annealings or shallow implantations. It also introduces a range of new dopant specific effects on diffusion, one of them being the fluorine effect. Fluorine is indeed widely used for boron implantation, through the implantation of the BF₂ species, as it serves two purposes: it allows to reduce the effective energy at which boron is implanted, allowing for shallow profiles, and it slows down the subsequent diffusion of boron further enabling the creation of a shallow junction. In this article we will first present the two fluorine models available with the CMOS diffusion model, and then perform a comparison of those in order to help the user chose the right model for their application.

II. MODELLING THE FLUORINE EFFECT ON DOPANT DIFFUSION

A. The Effect of Fluorine on Dopant Diffusion

There are many resources in literature discussing the effect of fluorine on dopant diffusion in silicon, especially on boron. Most of them agree on the fact that high concentration fluorine will hinder boron diffusion, up to a halting point. However, they do not agree on many points, like the eventual effect of amorphization during implantation or the exact mechanisms that are taking place to slow down the dopant diffusion. Some authors are suggesting that fluorine atoms will create clusters with vacancies, then providing a way to trap interstitials, while some others say that fluorine will directly bind with interstitials. In the Physical-based model section, we will discuss the choice that we had to make for our physical-based model, given that there is no clear consensus on how to build such a model.

B. Analytical Model

The analytical model is the simplest fluorine model. It reduces the diffusivity of boron in the presence of high fluorine concentration. It expresses the effective boron-interstitial pair diffusivity D_{BInt}^* as a function of the fluorine concentration:

$$D_{BInt}^* = D_{BInt} \times (1 + \alpha C_F) \times \left(\frac{1}{1 + \beta C_F} \right) \quad (1)$$

Here we are using the two Victory Process functions `dopingfactor` and `dopingdivisor`. The parameters α and β are calibration parameters. Their values, along with the function expression, can be set with two methods.

1. A MATERIAL statement
2. Directly in the open material database (smdb)

Example of a MATERIAL statement:

```
1 # Material statement
2 MATERIAL NAME=silicon
3   DIF.PARAM="streamfermiwithoutfield/BInt_A/D" \
4   DIF.PARAM="reactioncmos/BInt_A/D_BInt" \
5   DIF.PARAM="reactioncmos/Vac/D_BInt" \
6   DIF.PARAM="reactioncmos/B_L_A/D_BInt" \
7   PARAMETERUNIT="(cm3)(cm3)(cm2/s:eV:cm2/s:eV)" \
8   ALLPARAMETERSVALUE="(new) \
9   (linearmultiplier) \
10   (f1)(dopingfactor)(F)(constant)(1.5625E-22) \
11   (f2)(dopingdivisor)(F)(constant)(6.25E-21) \
12   (base)(arrheniustvostage)(1.817405E-08 / 4.661966E
-01 / 3.140957E-06 / 9.426641E-01)*"
```

Example of a setting from within the material database:

```
1 <D data="/s/routine/functiontype" unit="cm2/s" >
2   <functiontype data="/s/linearmultiplier"/>
3     <base data="opd:/ 1.35E-06 / 8.645745E-01" unit="cm2/s"/>
4     <f1>
5       <functiontype data="/s/dopingfactor"/>
6         <dopant data="/s/F"/>
7         <factor data="/d/ 1.5625E-22" unit="cm2/s"/>
8       </f1>
9       <f2>
10        <functiontype data="/s/dopingdivisor"/>
11        <dopant data="/s/F"/>
12        <divisor data="/d/ 6.25E-21" unit="cm2/s"/>
13      </f2>
14    </D>
```

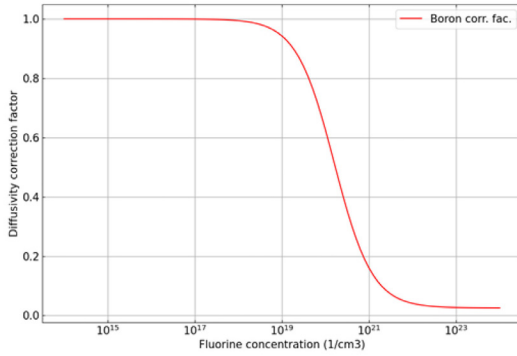


FIG. 1. Evolution of the diffusivity correction factor as a function of the total fluorine concentration.

The latest calibrated correction function is illustrated in Figure 1. We can see that for any concentration below 10^{19} cm^{-3} , fluorine will have close to no effect on boron diffusion. Then up to a concentration of 10^{21} cm^{-3} , the diffusivity will be greatly reduced. Above that threshold, boron will practically stop diffusing.

C. Physical-based Model: fluorine-FDT3

The physical-based model is a complex model that models the supposed reactions that take place in presence of fluorine. Literature tells us that boron uses interstitials to diffuse, so our model includes a mechanism that traps those. FDT stands for Formation, Dissolution and Trapping which are the three reactions modelled in this physical based model: the formation of fluorine-vacancy clusters, the trapping of interstitials by fluorine-vacancy clusters (or formation of fluorine-interstitial clusters) and the dissolution of the fluorine-vacancy clusters.

- Formation of fluorine vacancy clusters:



The corresponding reaction rate is expressed as follows:

$$k_{\text{FDT3}}^{\text{formation}} = k_2 C_{F_3V} - k_1 C_F C_V \quad (3)$$

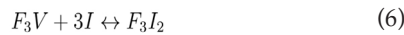
- Dissolution of fluorine vacancy clusters:



The corresponding reaction rate is expressed as follows:

$$k_{\text{FDT3}}^{\text{dissolution}} = k_2 C_F^3 - k_1 C_{F_3V} C_I \quad (5)$$

- Trapping of interstitials by fluorine vacancy clusters:



The corresponding reaction rate is expressed as follows:

$$k_{\text{FDT3}}^{\text{trapping}} = k_2 C_{F_3I_2} - k_1 C_{F_3V} C_I^3 \quad (7)$$

Where for each reaction, k_1 , k_2 are the respective forward and backward reaction rates. They are found in the reactioncmos section of the material database, and their names are the following:

- For the formation reaction:
k1_F3V_formation, k2_F3V_formation
- For the dissolution reaction:
k1_F3V_dissolution, k2_F3V_dissolution
- For the trapping reaction:
k1_F3V_trapping, k2_F3V_trapping

With this setup, the model clearly allows the fluorine to act as a sink for excess interstitials, which will lead to a decrease in the dopant diffusivity. The model was calibrated using data from the literature [1][2][3][4][5]. Another important aspect of this model is the definition of the initial conditions, which are the distributions of the species after the implantation. Here we see the effect of the amorphization playing a big role. At the moment:

- In the non amorphized zones, F_L is initialized to chemical F concentration while $F_3\text{Vac}$ and $F_3\text{Int}_2$ are set to 10^5 cm^{-3} .
- In the amorphized zones, $F_3\text{Vac}$ is initialized up to $5 \cdot 10^{20} \text{ cm}^{-3}$ while FL is set to 10^5 cm^{-3} and $F_3\text{Int}_2$ is set free.

The physical-based model can be enabled/disabled in-deck using the statement `METHOD dif.model.FLUORINEFDT3=ON`. Note that the empirical effect should then be switched off, either by removing or commenting out the corresponding `MATERIAL` statement, or by over-riding the open material database definition by using the appropriate `MATERIAL` statement.

III. COMPARISON OF THE TWO MODELS

In this section we will compare the analytical model and the FDT3-fluorine model previously presented. We will first discuss the differences obtained in terms of results as well as the differences in terms of simulation time.

A. Comparison of Results Obtained

Because the two models available for the fluorine effect are fundamentally different, they are likely to give different results, or at least in certain cases. In order to compare the results yielded by these models we have chosen to look at the concentration profiles of boron after various cases of implantations of BF2 and annealing conditions.

For fluorine concentrations below a certain threshold - typically 10^{20} cm^{-3} - the two models will produce the same results, for most implantation or annealing conditions, the illustrated in Figure 2. This is expected, given that the fluorine effect of slowing down the diffusion of boron is only attained at high concentrations. For these

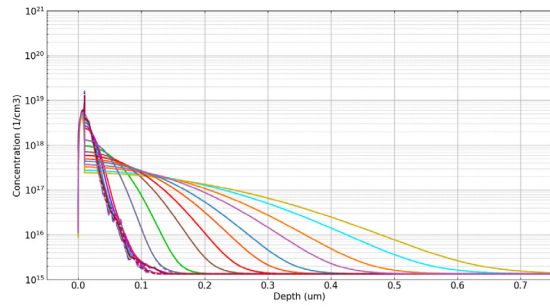


FIG. 2. Evolution of the boron profile for various diffusion times at 1000°C after a low dose (10^{13} cm^{-2}) BF2 implantation. The solid lines show the analytical model, the dashed lines show the physical-based model. Different colors indicate different annealing durations.

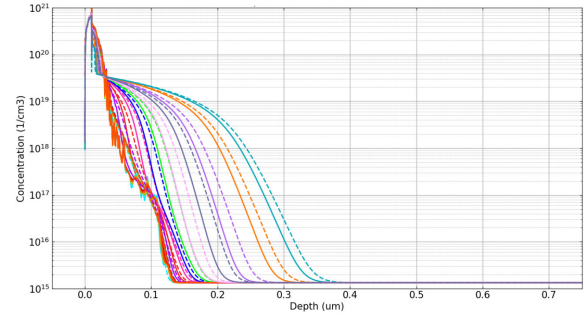


FIG. 4. Evolution of the boron profile for various diffusion times at 900°C after a high dose (10^{15} cm^{-2}) BF2 implantation. The solid lines show the analytical model, the dashed lines show the physical-based model. Different colors indicate different annealing durations.

high concentration cases, the physical-based model will overall result in more diffusion. The difference in diffusion will decrease with increasing annealing time, the two models converging eventually to the same result as transient diffusion effects are negligible compared to the equilibrium diffusion. This is illustrated in Figure 3. The difference in diffusion will also increase with decreasing temperature, mostly because the reaction rates get stronger at lower temperatures, which can be demonstrated by comparing figures 3 and 4.

B. Comparison of Simulation Times

The analytical model is obviously faster than the physical-based model, because of the reduced number of reactions to solve, so it is the obvious choice when there is no need for extreme precision on the results or if the case of application happens to have annealing and implantation conditions allowing the two model to yield similar results. Based on our benchmark of 1D and 2D cases, when using the FDT3 model, we can expect - on average - an increase of the simulation time between +100% and +300%. Note that it is possible for some cases to have even further increases in simulation time, depending on the process conditions.

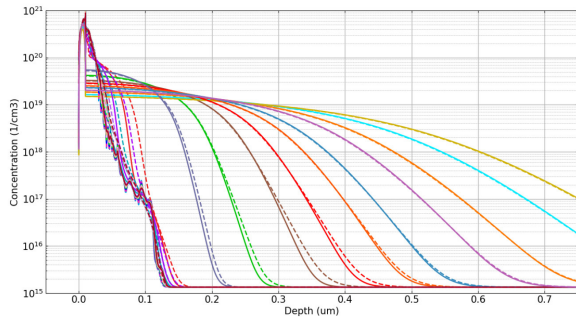


FIG. 3. Evolution of the boron profile for various diffusion times at 1000°C after a high dose (10^{15} cm^{-2}) BF2 implantation. The solid lines show the analytical model, the dashed lines show the physical-based model. Different colors indicate different annealing durations.

References

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